Re_L, Re_{L_2}

1977

ReH

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ReH_2
ReH_2^+

1991

0-4 Д177. Поверхности потенциальной энергии для внедрения Re и Re^+ в H_2. Potential energy surfaces for the insertion of Re and Re^+ into H_2 / Dai Dingguo, Balasubramanian K. // J. Chem. Phys.— 1991.— 95, № 6.— С. 4284—4295.— Англ.

Рассчитаны поверхности потенц. энергий (ППЭ) 12 электронных состояний ReH_2 и 13 электронных состояний ReH_2^+. Применялся метод ПАП—МКССП с включением $1{,}5 \cdot 10^6$ конфигураций. Получено, что в основных состояниях $Re(^6S)$ и $Re^+(^7S)$ не внедряются в H_2, в то время как возбужденные $Re(^6D)$ и $Re^+(^5G)$ спонтанно внедряются в H_2. Основное состояние ReH_2 высокоспиновое линейное $^6\Sigma_g^+$, а основное состояние ReH_2^+ — изогнутое $^5B_2$-состояние. Рассмотрены также некоторые низколежащие возбужденные состояния. Для ReH_2 и ReH_2^+ проявляются спин-орбитальные эффекты. Возбужденные состояния $ReH_2^+(^3B_2)$ и $(^1B_2)$ имеют ППЭ с двумя минимумами.

М.Л.

сф. 1992, N 4

ReH_2

1992

118: 132505h Theoretical study of rhenium hydride (ReH_2). Swang, O.; Faegri, K.; Gropen, O. (Dep. Chem., Univ. Oslo, N-0315 Oslo, Norway). *NATO ASI Ser., Ser. B* 1992, 283(Cluster Models Surf. Bulk Phenom.), 463-72 (Eng). The potential energy surfaces for a no. of quartet and sextet states of the ReH_2 were studied using ab initio CASSCF-CI and MCPF calcns. Different basis sets were applied; the treatment of correlation effects is discussed. The global energy min. of the ReH_2 is obtained with the H_2 mol. infinitely sepd. from the Re atom in its ^6S state. The most stable bound state is linear $^6\Sigma_g^+$ with $R(Re-H)$ = 1.88 Å 12.2 kcal/mol above the ref. state. A $^4B_1$ state with $R(Re-H)$ = 1.72 Å and a bond angle of 117 degrees is found 19.8 kcal/mol above the ref. These two energy min. are analogous to these of the H-Re-CH_3 system. The relationship between bonding energies and at. spectra is discussed.

теор. расчет

C.A. 1993, 118, N14

ReH

1993

118: 179024r Spectroscopic properties and potential energy curves for 30 electronic states of rhenium monohydride. Dai, Dingguo; Balasubramanian, K. (Dep. Chem., Arizona State Univ., Tempe, AZ 85287-1604 USA). *J. Mol. Spectrosc.* 1993, 158(2), 455–67 (Eng). Spectroscopic consts. and potential energy curves of 30 electronic states of the diat. ReH are computed using complete active space multiconfiguration SCF followed by first-order CI and multireference singles + doubles CI calcns. The second-order CI calcns. are made on four low-lying electronic states (T_e < 10,000 cm^{-1}). The authors also carry out relativistic CI calcns. including spin-orbit coupling to compute spin-orbit effects on the low-lying states of ReH. The ground state of ReH is found to be of $^7\Sigma^+$ symmetry (R_e = 1.82 Å, ω_e = 1611 cm^{-1}, D_e = 1.3 eV) with a very low-lying excited state of $^5\Sigma^+$ symmetry (T_e ~ 3000 cm^{-1}) in the absence of spin-orbit effects. The anal. of the wavefunctions and Mulliken populations reveals that all the low-lying electronic states of ReH are very ionic (Re^+H^-). The Re atom has an effective configuration of $6s^{1.15}6p^{0.45}5d^{5.01}$ and $6s^{1.75}6p^{0.05}5d^{5.09}$ in the $^7\Sigma^+$ and $^5\Sigma^+$ states, resp. The Re–H σ bond in the $^7\Sigma^+$ ground state has 45% Re(s), 16% Re(p), and 39% Re(d) character while in the $^5\Sigma^+$ state it has 60% Re(s), 2% Re(p), and 38% Re(d) character.

M.N., Norway
Q-mc

C.A. 1993, 118, N18

1994

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структурн. параметры, сил. пост. эл. сост., спин-орбит. взаимод., теор. расчет.

(сер.  MgH_2; III)